A Model for Heterogeneous Materials Including Phase Transformations

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An extension to the Method of Cells (MOC), which includes phase transformations of the constituents, has been developed. The MOC [1] is a homogenization technique that has demonstrated versatility. It has been applied to numerous composite materials and is applicable to general loading conditions. A diverse set of constitutive models has been used in the framework of the MOC both for the constituents and the interfaces. This approach is applicable to any ordered composite structure that can be idealized with a micro-structural unit cell (UC), which generates the entire composite through a periodic repetition. The macroscopic stress state, which is calculated for the UC, is taken to be the stress state at the corresponding location in the equivalent homogeneous continuum. The homogenized stress state is obtained as a solution for the mechanical response of the repeating UC to an applied macroscopic strain state, knowing the response of the constituents and the interfaces of the composite. The MOC has been implemented into engineering design analyses and used to model composite structures.

Many heterogeneous or composite materials contain constituents that undergo phase transformations during a deformation process. Examples include metal matrix composites that use titanium, which may be found in either the hexagonal close packed (hcp) alpha, the body-centered (bcc) beta, or the hexagonal (hex) omega phase, depending on the pressure and temperature of the composite. Similarly, polymer-bonded, high-explosive (PBX) materials contain a large percentage (approximately 95% by weight) of high-melting point explosive (HMX) and a polymer binder. HMX may be found in four solid phases.

An important reaction step in the initiation of HMX is the phase transformation from the beta (monoclinic) phase to the more reactive delta (hex) phase. In the conventional weapons community, depleted uranium alloys (DU) such as U-0.75 Ti have demonstrated effectiveness as kinetic energy, long-rod penetrators (LRPs). Unfortunately, uranium alloys present environmental problems ranging from fabrication to battle-field cleanup. Consequently, replacement materials have been pursued. Based on economic consideration and thermomechanical properties, tungsten heavy alloys (WHAs) have been considered as candidates for LRP applications. A typical WHA is composed of approximately 93 wt.% W, 5 wt.% Ni, and 2 wt.% Fe. The microstructure includes high strength, high melting point (T_{melt} ~ 3410 K), and rate-sensitive spherical grains of body-centered cubic (bcc) tungsten (W). The W particle size is roughly uniform (30 to 60 μm) and the microstructure is regular. There are no other phase transformations in the W grains between room temperature and the melting point. The W grains are dispersed in a softer, lower melting point (T_{melt} ~ 1750 K) face-centered cubic (fcc) W-Ni-Fe "matrix." The matrix material for a typical WHA has a composition of approximately 36 wt.% W, 45 wt.% Ni, and 19 wt.% Fe. Because of the low melting point of the matrix material, local melting is anticipated during a penetration event. For the above reasons, the ability to model phase transformations in composite materials remains an important problem.

A model for heterogeneous materials, which includes phase transformations, has been developed. The homogenization approach is a generalization of the MOC. An idealized UC is identified as a 3D rectilinear brick (Fig. 1). The UC contains eight subcells ($\alpha,\beta,\lambda=1,2$), which may correspond to different materials with different constitutive responses. The dimensions of the subcells are d_α, l_β, h_λ. It is assumed that the relative volume fractions of the constituents (i.e., subcell dimensions) remain constant during the deformation process. For this description, the density and temperature fields are assumed to be piecewise constant, and the velocity field

is assumed trilinear within each subcell. These approximations result in a consistent set of fields. Within subcells undergoing phase transformations, it is assumed that the velocity, temperature, and stress fields are equal for each of the phases. Separate mass, momentum, and energy equations are solved for the subcells using the constraints of periodic boundary conditions and continuity of displacements and tractions across the subcells. This approach is computationally efficient and may be coupled to a design analysis to provide the constitutive response for a composite material that may be used as part of an engineering structure.

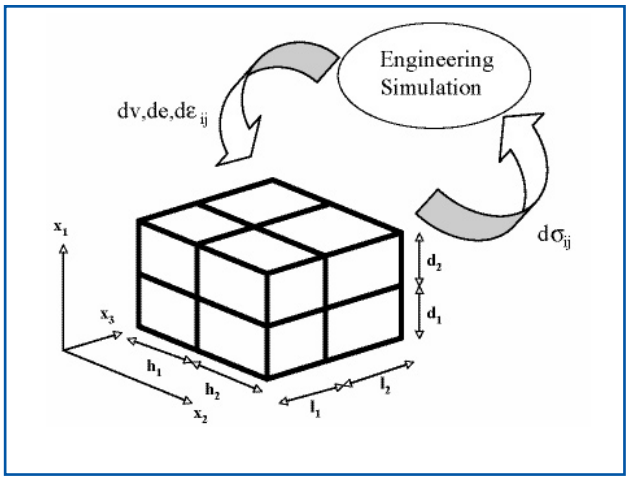

Figure 1— Representative Unit Cell used in the homogenization approach.

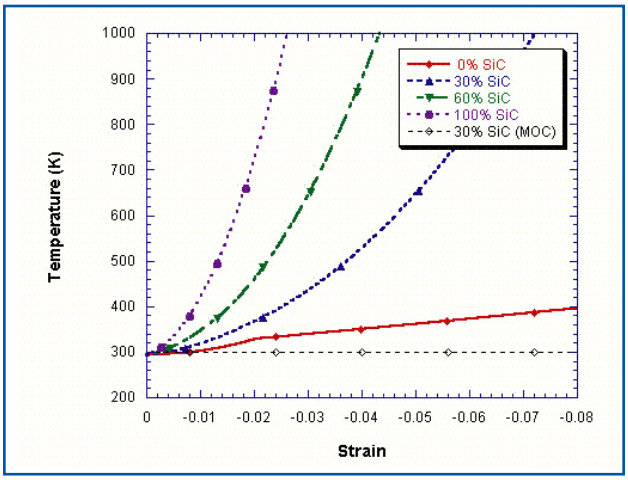

Figure 2— Biaxial compression simulation of a SiC-Ti particulate composite for two different compositions of SiC, temperature versus strain.

A simulation of a particulate composite composed of SiC particles embedded in a Ti matrix is provided in Fig. 2. Free energies for the Ti are obtained from electronic structure calculations [2]. A nonlinear elastic/plastic material model was used for the Ti. Nonlinear elasticity was modeled by obtaining the equation of state (EOS) directly from the free energies for Ti. Bodner-Partom plasticity was used for the inelastic response. The SiC was modeled as a simple nonlinear elastic material, using a Mie-Gruneisen EOS. Biaxial strain conditions were used in the simulations provided in Fig. 2. Simulations for four different compositions of SiC (0%, 30%, 60%, and 100%) are provided. A volume average temperature versus a volume average strain (ε_{11}) is plotted in the Fig. 2. In the figure, the phase transformation for the pure Ti (0% SiC) simulation begins and ends at a strains of about –0.0046 and –0.025, respectively. The phase transformation in Ti becomes less evident as larger amounts of SiC are added. In the pure SiC simulation, of course, there is no phase transformation present, during the deformation. Included in Fig. 2 is the response for a 30% SiC composition using the original MOC formulation, which excludes phase transformations. An isothermal response is obtained for the MOC simulation because the model does not include an energy equation.

Additional simulations have demonstrated the versatility and robustness of the model. Future applications, which address high-rate deformations of WHA and materials of interest to the nuclear weapons community, will be pursued.

[1] J. Aboudi, *Mechanics of Composite Materials: A Unified Micromechanical Approach*, (Elsevier, New York, NY 1991).

[2] C.W. Greeff, D.R. Trinkle, and R.C. Albers, "Shock-Induced α, ω Transition in Titanium," *J. Appl. Phys.* **90** (5) 2221 (2001).